



# Safer nuclear reactors could result from Los Alamos research

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## ***‘Loading-unloading’ effect of grain boundaries key to repair of irradiated metal***

LOS ALAMOS, New Mexico, March 25, 2010—Self-repairing materials within nuclear reactors may one day become a reality as a result of research by Los Alamos National Laboratory scientists.

In a paper appearing today in the journal *Science*, Los Alamos researchers report a surprising mechanism that allows nanocrystalline materials to heal themselves after suffering radiation-induced damage. Nanocrystalline materials are those created from nanosized particles, in this case copper particles. A single nanosized particle—called a grain—is the size of a virus or even smaller. Nanocrystalline materials consist of a mixture of grains and the interface between those grains, called grain boundaries.

When designing nuclear reactors or the materials that go into them, one of the key challenges is finding materials that can withstand an outrageously extreme environment. In addition to constant bombardment by radiation, reactor materials may be subjected to extremes in temperature, physical stress, and corrosive conditions. Exposure to high radiation alone produces significant damage at the nanoscale.

Radiation can cause individual atoms or groups of atoms to be jarred out of place. Each vagrant atom becomes known as an interstitial. The empty space left behind by the displaced atom is known as a vacancy. Consequently, every interstitial created also creates one vacancy. As these defects—the interstitials and vacancies—build up over time in a material, effects such as swelling, hardening or embrittlement can manifest in the material and lead to catastrophic failure.

Therefore, designing materials that can withstand radiation-induced damage is very important for improving the reliability, safety and lifespan of nuclear energy systems.

Because nanocrystalline materials contain a large fraction of grain boundaries—which are thought to act as sinks that absorb and remove defects—scientists have expected that these materials should be more radiation tolerant than their larger-grain counterparts. Nevertheless, the ability to predict the performance of nanocrystalline materials in extreme environments has been severely lacking because specific details of what occurs within solids are very complex and difficult to visualize.

Recent computer simulations by the Los Alamos researchers help explain some of those details.

In the Science paper, the researchers describe the never-before-observed phenomenon of a “loading-unloading” effect at grain boundaries in nanocrystalline materials.

This loading-unloading effect allows for effective self-healing of radiation-induced defects. Using three different computer simulation methods, the researchers looked at the interaction between defects and grain boundaries on time scales ranging from picoseconds to microseconds (one-trillionth of a second to one-millionth of a second).

On the shorter timescales, radiation-damaged materials underwent a “loading” process at the grain boundaries, in which interstitial atoms became trapped—or loaded—into the grain boundary. Under these conditions, the subsequent number of accumulated vacancies in the bulk material occurred in amounts much greater than would have occurred in bulk materials in which a boundary didn’t exist. After trapping interstitials, the grain boundary later “unloaded” interstitials back into vacancies near the grain boundary. In so doing, the process annihilates both types of defects—healing the material.

This unloading process was totally unexpected because grain boundaries traditionally have been regarded as places that accumulate interstitials, but not as places that release them. Although researchers found that some energy is required for this newly-discovered recombination method to operate, the amount of energy was much lower than the energies required to operate conventional mechanisms—providing an explanation and mechanism for enhanced self-healing of radiation-induced damage.

Modeling of the “loading-unloading” role of grain boundaries helps explain previously observed counterintuitive behavior of irradiated nanocrystalline materials compared to their larger-grained counterparts. The insight provided by this work provides new avenues for further examination of the role of grain boundaries and engineered material interfaces in self-healing of radiation-induced defects. Such efforts could eventually

assist or accelerate the design of highly radiation-tolerant materials for the next generation of nuclear energy applications.

The Los Alamos National Laboratory research team includes: Xian-Ming Bai, Richard G. Hoagland and Blas P. Uberuaga of the Materials Science and Technology Division; Arthur F. Voter, of the Theoretical Division; and Michael Nastasi of the Materials Physics and Applications Division.

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